Find the root of an equation

$$f(x^*) = 0 \qquad \text{for any } f(x)$$

$$\underset{\substack{\uparrow \\ \text{initial} \\ \text{estimate}}}{x_n} + \underset{\substack{\uparrow \\ \text{correction,} \\ \text{distance to } x^*}}{\epsilon_n} = x^*$$

$$f(x^*) = f(x_n + \epsilon_n) = f(x_n) + \epsilon_n f'(x_n) + \frac{1}{2}\epsilon_n^2 f'' + \frac{1}{6}\epsilon_n^3 f''' \cdots = 0$$

Solve for ϵ_n:

$$\epsilon_n \left[f'(x_n) + \frac{1}{2}\epsilon_n f'' + \frac{1}{6}\epsilon_n^2 f''' + \cdots \right] = -f(x_n)$$

$$\epsilon_n = -\frac{f(x_n)}{f'(x_n) + \frac{1}{2}\epsilon_n f'' + \frac{1}{6}\epsilon_n^2 f''' + \cdots}$$

Various estimates:

$$\epsilon_n^{(2)} = -\frac{f(x_n)}{f'(x_n)}$$

Newton's iteration

$$x_{n+1} = x_n + \epsilon_n^{(2)}$$

quadratic convergent

the # of correct digits double at every iteration.

$$\epsilon_n^{(3)} = -\frac{f(x_n)}{f'(x_n) + \frac{1}{2}\epsilon_n^{(2)} f''}$$

cubic convergent

$$\epsilon_n^{(4)} = -\frac{f(x_n)}{f'(x_n) + \frac{1}{2}\epsilon_n^{(3)} f'' + \frac{1}{6}\epsilon^{(3)2} f'''}$$

quartic convergent!

Example: $\sin(30^\circ) = \frac{1}{2}$

$\sin\left(\frac{\pi}{6}\right) = \frac{1}{2}$

Solve $\sin(x) = +\frac{1}{2}$ or $\underbrace{\sin(x) - \frac{1}{2}}_{f(x)} = 0$

$f(x) = 0$

$x^* = \frac{\pi}{6} \Rightarrow \pi = 6x^*$

$f'(x) = -\cos(x)$; $f''(x) = -\sin(x)$!

Mar 20-9:18 AM

Solve the radial Schrodinger Eq.

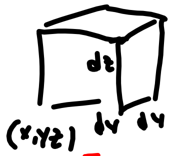
$$\left[-\frac{1}{2}\frac{\hbar^2}{m}\nabla^2 + V(r)\right]\psi^{(r,\theta,\phi)} = E\,\psi(r,\theta,\phi)$$

← time-independent Schrodinger Eq.

$r = \sqrt{x^2+y^2+z^2}$ or $\psi(x,y,z)$

replaces Newton's Second Law (time-dependent Schrodinger Eq.)

The prob. of finding the particle in the neighborhood of



$= dx\,dy\,dz$

$$P = |\psi(x,y,z)|^2\, dx\,dy\,dz$$

sq. wf = probability density fct.

distinction between classical mechanical complexity ↔ additive — 1 part. ~ 3 coor., 2 " ~ 6 coo.

quantum " " ↔ multiplicative — will.. " 3 with coord.

1 particle 1 D: $\psi(x) \leftrightarrow \psi_i \leftrightarrow 10$ grid values

$\psi(x,y) \leftrightarrow \psi_{ij} \leftrightarrow 10^2$ " "

$\psi(x,y,z) \leftrightarrow \psi_{ijk} \leftrightarrow 10^3$ " "

for N q. particle in 3D $\leftrightarrow (10^3)^N = 10^{3N}$

exponentially more complicated than class. Mech.

For the case of spherically symmetric pot. $V(r)$

$$\psi(\vec{r}) = \psi(r,\theta,\phi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\phi)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \qquad L^2 Y_{\ell m}(\theta,\varphi)$$

$$= \frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{\hbar^2}L^2(\theta,\varphi) \qquad = \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\varphi)$$

$$\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}$$

$$-\frac{1}{2}\frac{\hbar^2}{m}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}\right]R_{n\ell}(r) = E\, R_{n\ell}(r)$$

Note : $\frac{1}{r}\frac{\partial^2}{\partial r^2}(rf(r)) = \frac{1}{r}\left[0+2f'(r)+rf''(r)\right]$

therefore $-\frac{1}{2}\frac{\hbar^2}{m}\left[\cancel{\frac{1}{r}}\frac{\partial^2}{\partial r^2}(rR) - \frac{\ell(\ell+1)}{r^2}rR\right] = E\,R\,r$

define $u(r) = rR$ $\qquad -\frac{1}{2}\frac{\hbar^2}{m}\left[\frac{\partial^2}{\partial r^2}u - \frac{\ell(\ell+1)}{r^2}u\right] = Eu$

$+ V(r)u$

$$-\frac{1}{2}\frac{\hbar^2}{m}\frac{\partial^2}{\partial r^2}u + \underbrace{\left[\frac{1}{2}\frac{\hbar^2}{m}\frac{\ell(\ell+1)}{r^2}+V(r)\right]}_{V_{eff}(r)}u = Eu \qquad \epsilon = \frac{E}{(\hbar^2/m)}$$

$$v_{eff} = V_{eff}/(\hbar^2/m)$$

$$\boxed{-\frac{1}{2}\frac{\partial^2}{\partial r^2}u + v_{eff}(r)\,u = \epsilon u}$$

$$'' \; \frac{V(r)}{(\hbar^2/m)} + \frac{1}{2}\frac{\ell(\ell+1)}{r^2} \quad "v(r)"$$

"acceleration" $= \frac{\partial^2 u}{\partial r^2} = 2(v_{eff}-\epsilon)u$

$\frac{d^2u}{dt^2}$ $\Leftrightarrow$ equivalent to

$$= \underbrace{2\left(v(r)+\frac{1}{2}\frac{\ell(\ell+1)}{r^2}-\epsilon\right)}u$$

$$\frac{d^2u(t)}{dt^2} = f(t,\epsilon)\,u \qquad k(t,\epsilon) = -f(t,\epsilon)$$

$\hookrightarrow \ddot{u} = -k(t,\epsilon)\,u$

h o with a time + ϵ - dep. spring const. . .

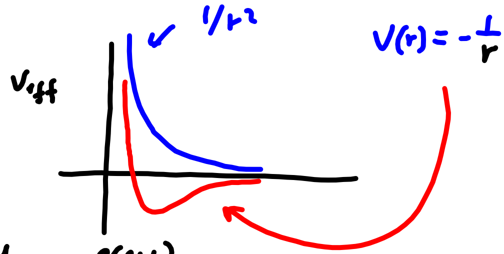
The "boundary" conditions for $u(r,\epsilon)$

$$\frac{d^2u}{dr^2} = f(r,\epsilon)\,u \qquad f = 2\left(V_{eff}(r) - \epsilon\right)$$

To determine ϵ, we need $\quad V_{eff}(r) = V(r) + \frac{\ell(\ell+1)}{2r^2}$

to know that $|V(r)|$ is not more singular than $\frac{1}{r^2}$

in the limit of $r \to 0$



$$\frac{d^2u}{dr^2} \cong \frac{\ell(\ell+1)}{r^2}\,u$$

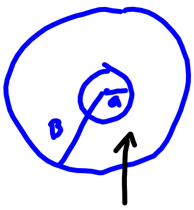
with solution $\quad u \propto r^{\alpha}$

$$\alpha(\alpha-1)\,r^{\alpha-2} = \frac{\alpha(\alpha-1)}{r^2}\,u = \frac{\ell(\ell+1)}{r^2}\,u$$

$$\alpha(\alpha-1) = \ell(\ell+1) \quad \Longrightarrow \quad \alpha - 1 = \ell \;\Rightarrow\; \alpha = \ell + 1$$

solutions

$$\alpha = -\ell$$



$A r^{\ell+1} + \frac{B}{r^{\ell}}$

$u(r) \to r^{\ell+1}$ as $r \to 0$ regular solution

$$\boxed{u(0) = 0}$$

singular at $r = 0$ irregular solution.

Mar 22-9:31 AM

The "eigen condition" for determining ϵ

$r \to \infty$ if $v(r) \to 0$ then

$$\frac{d^2u}{dr^2} = -2\epsilon u \qquad \text{take } u = e^{\alpha r}$$

$$\alpha^2 e^{\alpha r} = -2\epsilon e^{\alpha r} \qquad \alpha^2 = -2\epsilon$$

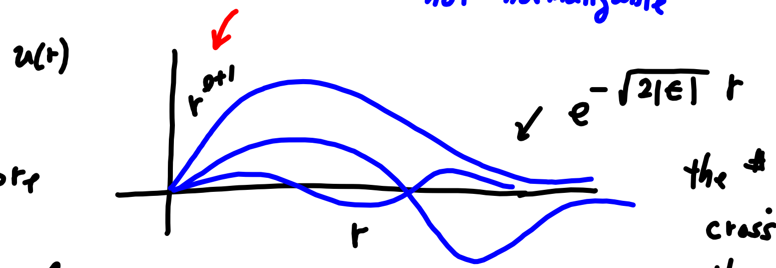
bound state $\epsilon < 0$

$$\alpha = \sqrt{2|\epsilon|}$$

$$\underset{r\to\infty}{u(r)} = A e^{-\sqrt{2|\epsilon|}\, r} + \cancel{\beta e^{+\sqrt{2|\epsilon|}\, r}}$$

not normalizable

for all $v(r) \to 0$, $r \to \infty$



therefore

$\epsilon_{n_r, \ell}$

↖ # of zero-crossing

the # of zero crossing gives the radial quantum number

Solving u numerically

$u \to$ "x"
$r \to$ "t"

$$\frac{d^2u}{dr^2} = f(r,\epsilon)\,u \qquad f = 2V_{eff} - 2\epsilon$$

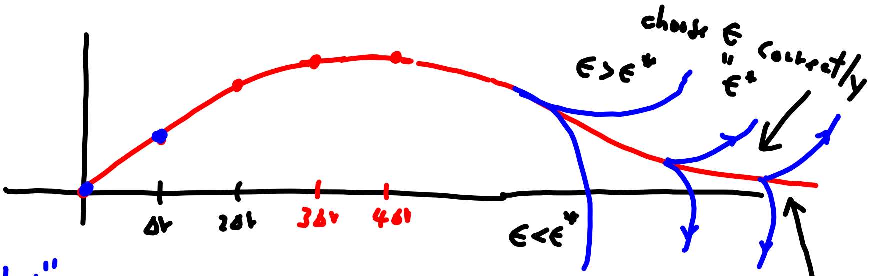
Verlet algorithm

$$u(r+\Delta r) = u(r) + \Delta r\, u'(r) + \tfrac{1}{2}\Delta r^2 u''(r) + \cdots$$
$$u(r-\Delta r) = \;\;'' \;\; - \qquad + \tfrac{1}{2}\Delta r^2 u''(r) + \cdots$$

$$u(r+\Delta r) + u(r-\Delta r) = 2u(r) + \Delta r^2 u''(r)$$

$$\boxed{u(r+\Delta r) = 2u(r) - u(r-\Delta r) + \Delta r^2 f(r,\epsilon)\,u(r)}$$

Since $u(r) \sim r^{\ell+1}$

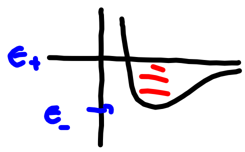


"shooting method" $\rightarrow$ Guess ϵ, increase or decrease, so that this is achieved.

1) Hard wall - method.

Given ϵ in the range $[\epsilon_-, \epsilon_+]$

in the case of hydrogen $[-\frac{1}{2}, 0]$



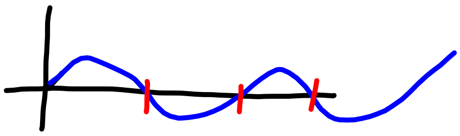
for a given ℓ

Given.

do $i = 1, 1000$

$\Delta\epsilon = 0.001$

$\epsilon = \epsilon_- + i\Delta\epsilon$



whenever u crosses zero, i.e. $u(k\Delta r)\,u((k+1)\Delta r) < 0$

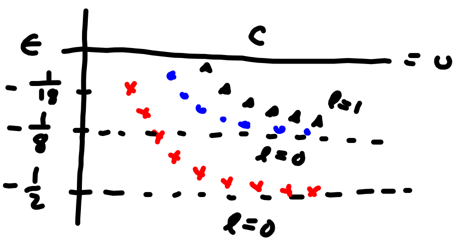
set the crossing pt $c = (k+\frac{1}{2})\Delta r$

out put (ϵ, c) at a given ℓ

end do

Every crossing → wf of the pot. with an infinite wall at c.

Plot.



$-\frac{1}{2n^2}$

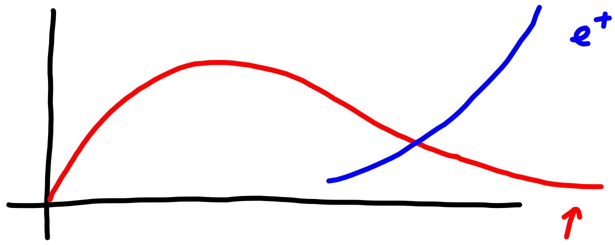
To determine ϵ, u accurately

$\rightarrow$ Killingbeck's method

$\swarrow$ growing solution

$e^{+\sqrt{2|\epsilon|}\,r}$

however, inward integration is stable



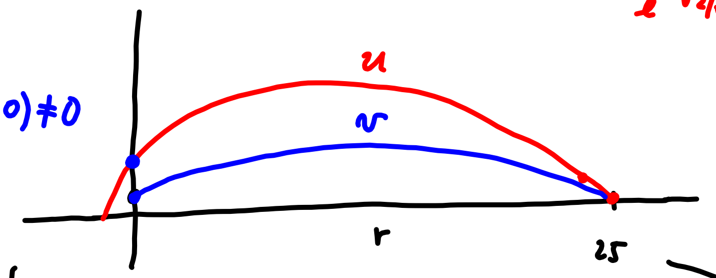
outward integration is instrinsically unstable.

$\uparrow$

$e^{-\sqrt{2|\epsilon|}\,r}$

at $u(\epsilon,0)\neq 0$

$\uparrow$



given an initial ϵ, + ℓ,

need to find $u(\epsilon^*,0)=0$

$\Delta r = \frac{25}{1000}$

recall $f(x^*)=0$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

$\uparrow$

$$\epsilon_{n+1} = \epsilon_n - \frac{u(\epsilon_n,0)}{u'(\epsilon_n,0)} \leftarrow \quad u' = \frac{du}{d\epsilon}$$

$$\left\{\begin{array}{l} u(r-\Delta r) = 2u(r) - u(r+\Delta r) + \Delta r^2 f(r,\epsilon)\,u(r) \quad '' \; v(\epsilon_n,0) \\ v(r-\Delta r) = 2v(r) - v(r+\Delta r) \end{array}\right.$$

integrate both inward

$$+ \Delta r^2 f(r,\epsilon)\,v(r)$$

$$+ \Delta r^2 \underbrace{\frac{\partial f}{\partial \epsilon}}_{-2} u(r)$$

$$f(r,\epsilon) = 2V(r) - 2\epsilon + \frac{\ell(\ell+1)}{r^2}$$

Only a few Newton's iteration will determine ϵ_n to double precision.

Can improve on Newton's iteration for faster convergence.

cubic, quartic